

104499

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: Jeffrey E. Russell Examiner #: 62785 Date: 9-24-2003
 An Unit: 1654 Phone Number 308-3970 Serial Number: 101088078
 Mail Box and Bldg/Room Location: CM1-11013/CM1-9807 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

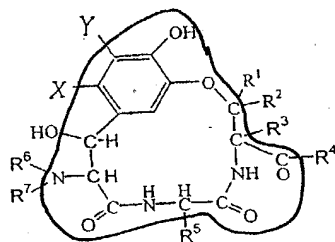
Title of Invention: Anticancer Agent And Method Of Treatment Of Cancer

Inventors' (please provide full names): J. Edgar

Earliest Priority Filing Date: 7-22-2002

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

Please search the following partial structure, ignoring the sidechain identities.



(1)

Please limit any hits using the keywords cancer, tumor, carcinoma, ~~conjugated?~~ conjugated?

Thank you.

JER

Point of Contact
 P. Sheppard
 Telephone number: (703) 308-4499

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Type of Search

Vendors and cost where applicable

Searcher: _____	NA Sequence (#) _____	STN: _____
Searcher Phone #: _____	AA Sequence (#) _____	Dialog: _____
Searcher Location: _____	Structure (#) _____	Questel/Orbit: _____
Date Searcher Provided: _____	Bibliographic: _____	Dr. Link: _____
Date Completed: <u>9/25/03</u>	Litigation: _____	Levy's News: _____
Searcher Prep & Review Time: _____	Fulltext: _____	Sequence Systems: _____
Client Prep Time: _____	Patent Family: _____	WWW Internet: _____
Online Time: _____	Other: _____	Other Specified: _____

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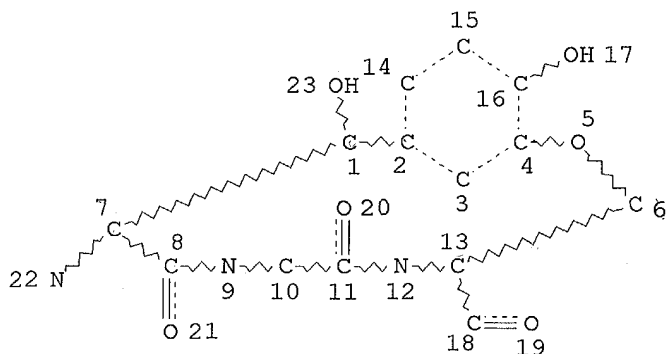
FILE COVERS 1907 - 25 Sep 2003 VOL 139 ISS 13

FILE LAST UPDATED: 24 Sep 2003 (20030924/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

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L1 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

MLEVEL IS CLASS AT 14 15 16

DEFAULT ECLEVEL IS LIMITED

ECOUNT IS UNLIMITED AT 14 15 16

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE

L3 22 SEA FILE=REGISTRY SSS FUL L1

L4 65 SEA FILE=HCAPLUS ABB=ON PLU=ON L3

L5 10 SEA FILE=HCAPLUS ABB=ON PLU=ON L4 AND (?CANCER? OR ?TUMOR?
OR ?CARCIN? OR ?MALIGNA? OR ?NEOPLAS? OR CONJUGAT?)

Russel 10_088078

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L5 ANSWER 1 OF 10 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2002:869496 HCAPLUS

DOCUMENT NUMBER: 137:363033

TITLE: Peptidomimetic modulators of cell adhesion

INVENTOR(S): Gour, Barbara J.; Blaschuk, Orest W.; Ali, Anmar; Ni, Feng; Chen, Zhigang; Michaud, Stephanie D.; Wang, Shoameng; Hu, Zengjian

PATENT ASSIGNEE(S): Can.

SOURCE: U.S. Pat. Appl. Publ., 309 pp., Cont.-in-part of U.S. Ser. No. 491,078.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2002168761	A1	20021114	US 2001-769145	20010124
PRIORITY APPLN. INFO.:			US 2000-491078	A2 20000124

OTHER SOURCE(S): MARPAT 137:363033

AB Peptidomimetics of cyclic peptides, and compns. comprising such peptidomimetics are provided. The peptidomimetics have a three-dimensional structure that is substantially similar to a three-dimensional structure of a cyclic peptide that comprises a cadherin cell adhesion recognition sequence HAV. Methods for using such peptidomimetics for modulating cadherin-mediated cell adhesion in a variety of contexts are also provided.

IT **351858-59-8**, Aspartic acid, (.beta.R)-3-chloro-.beta.,5-dihydroxy-N-methyl-D-tyrosyl-3,4-didehydro-L-valyl-3-hydroxy-L-isoleucyl-3,4-didehydro-L-prolyl-2,3-didehydroisoleucyl-2,3-didehydro-, cyclic (15.fwdarw.3)-ether

RL: BSU (Biological study, unclassified); PAC (Pharmacological activity); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)

(peptidomimetic modulators of cadherin-mediated cell adhesion for therapeutic use in relation to three-dimensional structure)

L5 ANSWER 2 OF 10 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2001:545724 HCAPLUS

DOCUMENT NUMBER: 135:147398

TITLE: Peptidomimetic modulators of cell adhesion

INVENTOR(S): Gour, Barbara J.; Blaschuk, Orest W.; Ali, Anmar; Ni, Feng; Chen, Zhigang; Michaud, Stephanie Denise; Wang, Shoameng; Hu, Zengjian

PATENT ASSIGNEE(S): Adherex Technologies, Inc., Can.

SOURCE: PCT Int. Appl., 416 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001053331	A2	20010726	WO 2001-US2508	20010124

Russel 10 088078

WO 2001053331 A3 20020711
WO 2001053331 C2 20021031

W:	AE,	AG,	AL,	AM,	AT,	AU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,	
	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,	HR,	
	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,	LS,	LT,	
	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	PL,	PT,	RO,	RU,	
	SD,	SE,	SG,	SI,	SK,	SL,	TJ,	TM,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,	VN,	
	YU,	ZA,	ZW,	AM,	AZ,	BY,	KG,	KZ,	MD,	RU,	TJ,	TM					
RW:	GH,	GM,	KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZW,	AT,	BE,	CH,	CY,	
	DE,	DK,	ES,	FI,	FR,	GB,	GR,	IE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,	BF,	
	BJ,	CF,	CG,	CI,	CM,	GA,	GN,	GW,	ML,	MR,	NE,	SN,	TD,	TG			

PRIORITY APPLN. INFO.: US 2000-491078 A 20000124

OTHER SOURCE(S) : MARPAT 135:147398

AB Peptidomimetics of cyclic peptides, and compns. comprising such peptidomimetics are provided. The peptidomimetics have a three-dimensional structure that is substantially similar to a three-dimensional structure of a cyclic peptide that comprises a cadherin cell adhesion recognition sequence HAV. Methods for using such peptidomimetics for modulating cadherin-mediated cell adhesion in a variety of contexts are also provided.

IT 351858-59-8

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(peptidomimetic modulators of cell adhesion)

L5 ANSWER 3 OF 10 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 2001:247198 HCAPLUS

DOCUMENT NUMBER: 134:261242

TITLE: Phomopsin **anticancer** agents and treatment
method

INVENTOR(S) : Edgar, John Alexander

PATENT ASSIGNEE(S): Commonwealth Scientific and Industrial Research
Organisation, Australia

SOURCE: PCT Int. Appl., 28 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.		KIND	DATE	APPLICATION NO.		DATE	
WO	2001022986	A1	20010405	WO	2000-AU1193	20000929	
W:	AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM						
RW:	GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG						
EP	1216051	A1	20020626	EP	2000-969057	20000929	
R:	AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL						
JP	2003510287	T2	20030318	JP	2001-526195	20000929	

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PRIORITY APPLN. INFO.:

AU 1999-3148 A 19990929
WO 2000-AU1193 W 20000929

OTHER SOURCE(S): MARPAT 134:261242

AB A method of treatment of a patient suffering from **cancer** comprises administering to the patient an effective amt. of a phomopsin.

IT **64925-80-0P**, Phomopsin A

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PUR (Purification or recovery); RCT (Reactant); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(phomopsin **anticancer** agents)

IT **89085-54-1P**, Phomopsinamine A **332094-78-7P**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(phomopsin **anticancer** agents)

IT **110580-02-4**

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(phomopsin **anticancer** agents)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 4 OF 10 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1998:753888 HCAPLUS

DOCUMENT NUMBER: 130:152150

TITLE: Towards a commercial vaccine against lupinosis

AUTHOR(S): Edgar, J. A.; Than, K. A.; Payne, A. L.; Anderton, N.; Baell, J.; Cao, Y.; Cockrum, P. A.; Michalewicz, A.; Stewart, P. L.; Allen, J. G.

CORPORATE SOURCE: CSIRO Division of Animal Health, Australian Animal Health Laboratory, Geelong, 3220, Australia

SOURCE: Toxic Plants and Other Natural Toxicants, [Proceedings of the International Symposium on Poisonous Plants], 5th, San Angelo, Tex., May 18-23, 1997 (1998), Meeting Date 1997, 196-200. Editor(s): Garland, Tam; Barr, A. Catherine. CAB International: Wallingford, UK.
CODEN: 66ZXA6

DOCUMENT TYPE: Conference; General Review

LANGUAGE: English

AB A review and discussion with 4 refs. Lupinosis is caused by phomopsin mycotoxins produced by a fungus, *Diaporthe toxica*, that infects and colonizes lupines. The authors discuss an immunogen made by **conjugating** phomopsin A to keyhole limpet hemocyanin as an effective vaccine against the livestock poisoning disease lupinosis. A considerable amt. of work has been conducted since then, aimed at converting the exptl. vaccine into a com. product. Topics included are: prodn. and **conjugation** of phomopsins; min. ED of phomopsin A per injection; and vaccination protocol and protection studies.

IT **64925-80-0**, Phomopsin A

RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(com. vaccine against lupinosis in livestock)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 5 OF 10 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1998:297640 HCAPLUS

DOCUMENT NUMBER: 129:38537
 TITLE: Isolation and structure of an antimitotic cyclic peptide, ustiloxin F: chemical interrelation with a homologous peptide, ustiloxin B
 AUTHOR(S): Koiso, Yukiko; Morisaki, Naoko; Yamashita, Yukiko; Mitsui, Yukiko; Shirai, Ryuichi; Hashimoto, Yuichi; Iwasaki, Shigeo
 CORPORATE SOURCE: Institute of Molecular and Cellular Biosciences, The University of Tokyo, Tokyo, 113-0032, Japan
 SOURCE: Journal of Antibiotics (1998), 51(4), 418-422
 CODEN: JANTAJ; ISSN: 0021-8820
 PUBLISHER: Japan Antibiotics Research Association
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 AB Ustiloxin F, a microtubule inhibitor, was isolated as a minor metabolite of Ustilaginoidea virens. The structure was detd. from the spectral data and by chem. interrelation to ustiloxin B through reductive removal of the sulfoxide-contg. side chain of ustiloxin B to give ustiloxin F. Ustiloxin F inhibited microtubule assembly with an IC50 value of 10.3 .mu.M.
 IT 143557-93-1, Ustiloxin A
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (conversion of ustiloxin A to ustiloxin D)
 IT 158243-18-6P, Ustiloxin D
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (conversion of ustiloxin A to ustiloxin D)
 IT 151841-41-7, Ustiloxin B
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (conversion of ustiloxin B to ustiloxin F)
 IT 208392-87-4P, Ustiloxin F
 RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); SPN (Synthetic preparation); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)
 (isolation, mol. structure and biol. activity of ustiloxin F)
 REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 6 OF 10 HCAPLUS COPYRIGHT 2003 ACS on STN
 ACCESSION NUMBER: 1995:698898 HCAPLUS
 DOCUMENT NUMBER: 123:283737
 TITLE: Ustiloxins manufacture with Ustilaginoidea as **neoplasm** inhibitors
 INVENTOR(S): Iwasaki, Shigeo; Koiso, Kuniko
 PATENT ASSIGNEE(S): Sankyo Co, Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07101983	A2	19950418	JP 1993-251327	19931007
PRIORITY APPLN. INFO.:			JP 1993-251327	19931007

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Ustiloxins, ustiloxin C (I) and D (II), are manufd. by culturing Ustilaginoidea virens. I and II inhibit polymn. of tublin and useful as **neoplasm** inhibitors. The physicochem. characteristics of I and II and the physiol. and morphol. characteristics of Ustilaginoidea virens were given.

IT **158243-18-6P**, Ustiloxin D **158274-98-7P**, Ustiloxin C
 RL: BPN (Biosynthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
 (ustiloxins manuf. with Ustilaginoidea as **neoplasm** inhibitors)

L5 ANSWER 7 OF 10 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1994:473249 HCAPLUS

DOCUMENT NUMBER: 121:73249

TITLE: Increase in the chemically-induced differentiation of human leukemia cell lines by tubulin disruptors

AUTHOR(S): Nakajima, Osamu; Sugishita, Yasuko; Hashimoto, Yuichi; Iwasaki, Shigeo

CORPORATE SOURCE: Inst. Mol. Cellular Biosciences, University Tokyo, Tokyo, 113, Japan

SOURCE: Biological & Pharmaceutical Bulletin (1994), 17(5), 742-4

CODEN: BPBLEO; ISSN: 0918-6158

DOCUMENT TYPE: Journal

LANGUAGE: English

AB The effect of various structural functional tubulin disruptors (including colchicine-type disruptors, vinblastine, rhizoxin, maytansine, peptide-type disruptors, and taxol) on the chem. induced differentiation of human leukemia cell lines (HL-60 and K562) was examd. As differentiation-inducing agents, 12-O-tetradecanoylphorbol-13-acetate (TPA) was used for the differentiation of both HL-60 and K562 to monocyte/macrophages, retinoids were used for the differentiation of HL-60 to mature granulocytes, and hemin was used for the erythroid differentiation of K562. All the tubulin disruptors investigated increased the chem.-induced differentiation of HL-60 and K562 cell lines to the cognate mature cell types, regardless of the nature of the differentiation.

IT **64925-80-0**, Phomopsin A **143557-93-1**, Ustiloxin
 RL: BIOL (Biological study)
 (chem. induced leukemia cell differentiation increase by, of humans, as tubulin disruptor)

L5 ANSWER 8 OF 10 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1994:158265 HCAPLUS

DOCUMENT NUMBER: 120:158265

TITLE: Mitotic poison, ustiloxin, from false smut balls on rice plant, and a related peptide: structure and activities

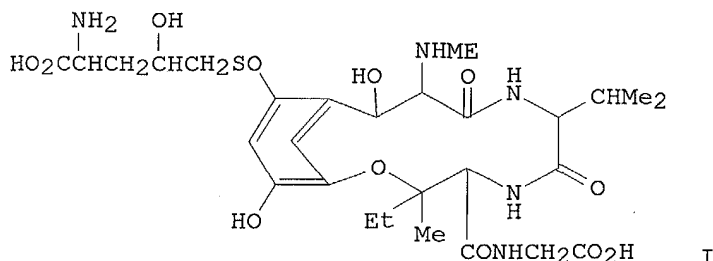
AUTHOR(S): Koiso, Y.; Li, Y.; Kobayashi, H.; Natori, M.; Hashimoto, Y.; Iwasaki, S.; Fujita, Y.; Sonoda, R.; Yaegashi, H.; et al.

CORPORATE SOURCE: Inst. Appl. Microbiol., Univ. Tokyo, Tokyo, 113, Japan

SOURCE: Tennen Yuki Kagobutsu Toronkai Koen Yoshishu (1992), 34th, 566-573

DOCUMENT TYPE:
LANGUAGE:
GI

CODEN: TYKYDS
Journal
Japanese



AB The false smutted balls growing parasitically on panicles of rice plant (Ina-koji) are caused by a pathogen, *Ustilaginoidea virens*. Ingestion of such rice plant caused poisoning to domestic animals. Deep red pigments, ustilaginoidins, have been isolated from the ether ext. of the balls but these compds. were not the causative compds. as the phytotoxin or the mycotoxin. The authors report on the isolation, the structure and the biol. activities of a toxin, ustiloxin(I), which was isolated from the water ext. of the balls, as well as on the mode of action of a mycotoxin, phomopsin A, whose structure is closely related to that of I. Abs. structure of I was detd. to be a unique cyclic tetra peptide contg. a 13-membered ring including an ether linkage, by combination of spectroscopic, amino acid and X-ray crystallog. analyses. The compd. induces an abnormal swelling of the seedling roots. Such a symptom is induced also by rhizoxin, a potent antimitotic agent. I strongly inhibits the polymn. of porcine brain tubulin and also shows potent cytotoxicity against broad range of **tumor** cells. Phomopsin A, structurally similar to I, is also a potent antimitotic agent and inhibits tubulin polymn. Its binding site on porcine brain tubulin was identical with that of rhizoxin and maytansine. Phomopsin A does not bind to fungal tubulin and shows no antifungal activity, whereas rhizoxin and maytansine are potent fungicides.

IT **64925-80-0**, Phomopsin A **143557-93-1**, Ustiloxin
RL: BIOL (Biological study)
(mol. structure and biol. activities of)

L5 ANSWER 9 OF 10 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1994:14886 HCAPLUS

DOCUMENT NUMBER: 120:14886

TITLE: Manufacture of tetrapeptide derivative, ustiloxin A or B, with *Ustilaginoidea virens* (Cooke) Takahashi SANK 15391 and synthesis of derivative thereof as **antitumor** agent

INVENTOR(S): Iwasaki, Shigeo; Koiso, Kuniko; Kobayashi, Tomowo

PATENT ASSIGNEE(S): Sankyo Co., Ltd., Japan

SOURCE: PCT Int. Appl., 28 pp.

CODEN: PIXXD2

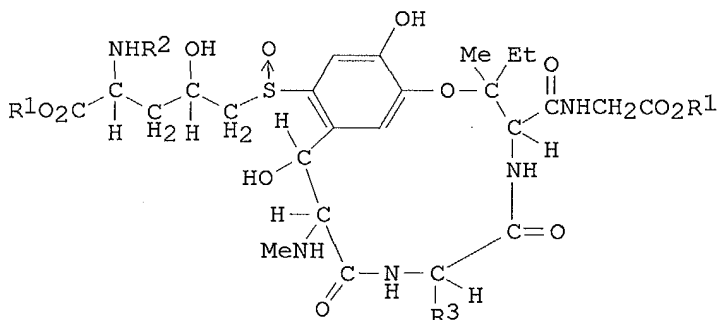
DOCUMENT TYPE: Patent

Russel 10_088078

LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9314111	A1	19930722	WO 1993-JP18	19930108
RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
JP 05345796	A2	19931227	JP 1993-988	19930107
JP 3276187	B2	20020422		
AU 9332665	A1	19930803	AU 1993-32665	19930108
PRIORITY APPLN. INFO.:			JP 1992-1139	A 19920108
			WO 1993-JP18	A 19930108

GI



I

AB The title peptide derivs. (I; R1 = H, C1-5 alkyl; R2 = H, C2-6 alkyl, aliph. acyl; R3 = Me, Pr) or their salts are prepd. Thus, ustiloxin A (I; R1 = R2 = H, R3 = Me) and ustiloxin B I (R1 = R2 = H, R3 = Pr) were isolated from the water ext. of false smut balls caused by Ustilaginoidea virens on the panicles of rice plants. Esterification of ustiloxin A with 12% methanolic HCl at 4.degree. overnight gave ustiloxin A di-Me ester dihydrochloride. Ustiloxin A and B showed IC50 of 2.46 and 2.85 .mu.g/mL, resp., against stomach **cancer** MKN-1 cells, and 0.656 and 1.38 .mu.g/mL, resp., against breast **cancer** MCF-7 cells, which were as potent as 5-fluorouracil.

IT 143557-93-1 151841-41-7, Ustiloxin B

RL: PROC (Process)

(from Ustilaginoidea virens-infected rice panicles, isolation of, as **antitumor** agent)

IT 151586-08-2P, Ustiloxin A dimethyl ester dihydrochloride

151586-09-3P

RL: THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of, as **antitumor** agent)

L5 ANSWER 10 OF 10 HCAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1990:470858 HCAPLUS

DOCUMENT NUMBER: 113:70858

TITLE: Dolastatin 10, a powerful cytostatic peptide derived from a marine animal. Inhibition of tubulin

polymerization mediated through the vinca alkaloid binding domain

AUTHOR(S): Bai, Ruoli; Pettit, George R.; Hamel, Ernest
CORPORATE SOURCE: Lab. Biochem. Pharmacol., Natl. Cancer Inst.,
Bethesda, MD, 20892, USA
SOURCE: Biochemical Pharmacology (1990), 39(12), 1941-9
CODEN: BCPCA6; ISSN: 0006-2952
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Dolastatin 10, a cytostatic peptide contg. several unique amino acid subunits, was isolated from the marine shell-less mollusk *Dolabella auricularia*. Since preliminary studies demonstrated that dolastatin 10 inhibited tubulin polymn. and the binding of radiolabeled vinblastine to tubulin, an initial characterization of the properties of dolastatin 10 included a comparison to other antimitotic drugs interfering with vinca alkaloid binding to tubulin (vinblastine, maytansine, rhizoxin, and phomopsin A). Dolastatin 10 inhibited the growth of L1210 murine leukemia cells in culture, with a concordant rise in the mitotic index, and its IC50 value for cell growth was 0.5 nM. Comparable values for the other drugs were 0.5 nM for maytansine, 1 nM for rhizoxin, 20 nM for vinblastine, and 7 .mu.M for phomopsin A. IC50 values were also obtained for the polymn. of purified tubulin in glutamate: 1.2 .mu.M for dolastatin 10, 1.4 .mu.M for phomopsin A, 1.5 .mu.M for vinblastine, 3.5 .mu.M for maytansine, and 6.8 .mu.M for rhizoxin. Dolastatin 10 and vinblastine were comparable in their effects on microtubule assembly dependent on microtubule-assocd. proteins. Preliminary studies indicated that dolastatin 10, like vinblastine, causes formation of a cold-stable tubulin aggregate at higher drug concns. Results confirmed that rhizoxin, phomopsin A, and maytansine also inhibit the binding of radiolabeled vinblastine and vincristine to tubulin. Dolastatin 10 and phomopsin A were the strongest inhibitors of these reactions, and rhizoxin the weakest. Dolastatin 10, phomopsin A, maytansine, vinblastine, and rhizoxin all inhibited tubulin-dependent GTP hydrolysis. The greatest inhibition of hydrolysis was obsd. with dolastatin 10 and phomopsin A, and the least inhibition with rhizoxin.

IT 64925-80-0, Phomopsin A
RL: BIOL (Biological study)
(tubulin polymn. inhibition by dolastatin 10 vs.)

=> file reg

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STRUCTURE FILE UPDATES: 24 SEP 2003 HIGHEST RN 592465-25-3
DICTIONARY FILE UPDATES: 24 SEP 2003 HIGHEST RN 592465-25-3

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Russel 10_088078

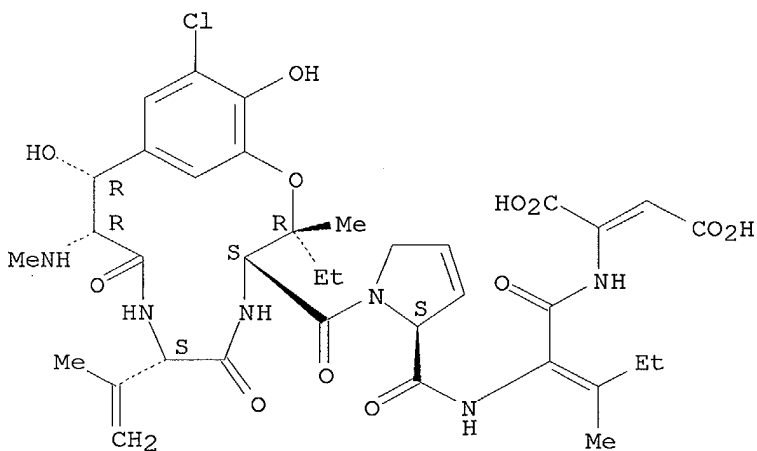
Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> d ide can l3 1-22

L3 ANSWER 1 OF 22 REGISTRY COPYRIGHT 2003 ACS on STN
RN 351858-59-8 REGISTRY
CN Aspartic acid, (.beta.R)-3-chloro-.beta.,5-dihydroxy-N-methyl-D-tyrosyl-3,4-didehydro-L-valyl-3-hydroxy-L-isoleucyl-3,4-didehydro-L-prolyl-2,3-didehydroisoleucyl-2,3-didehydro-, cyclic (15.fwdarw.3)-ether (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
MF C36 H45 Cl N6 O12
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.
Double bond geometry unknown.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 137:363033

REFERENCE 2: 135:147398

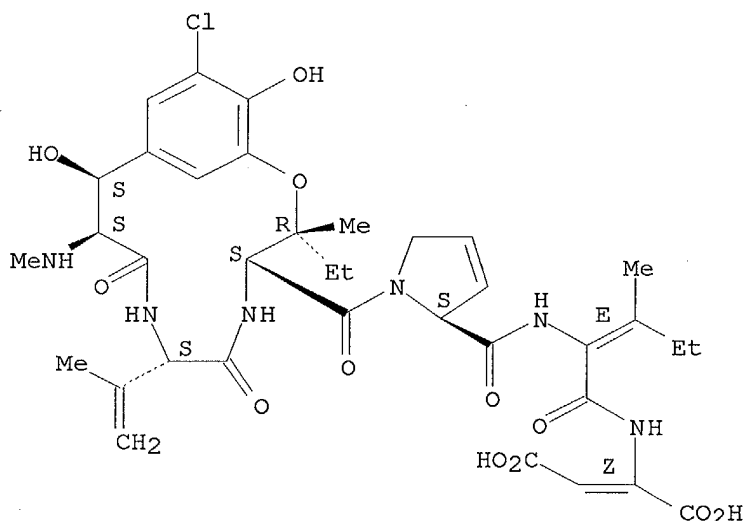
L3 ANSWER 2 OF 22 REGISTRY COPYRIGHT 2003 ACS on STN
RN 332094-78-7 REGISTRY
CN Aspartic acid, (.beta.S)-3-chloro-.beta.,5-dihydroxy-N-methyl-L-tyrosyl-

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3,4-didehydro-L-valyl-3-hydroxy-L-isoleucyl-3,4-didehydro-L-prolyl-(2E)-
2,3-didehydroisoleucyl-2,3-didehydro-, cyclic (15.fwdarw.3)-ether, (2Z)-
(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH
MF C36 H45 Cl N6 O12
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.
Double bond geometry as shown.



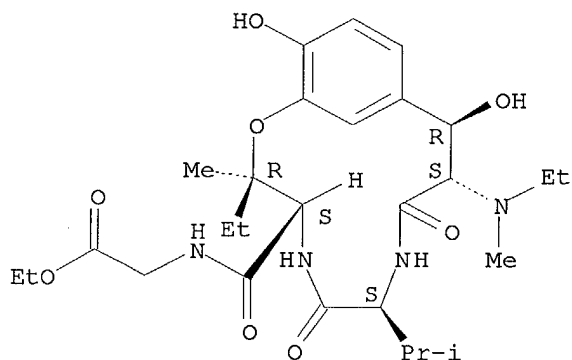
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 134:261242

L3 ANSWER 3 OF 22 REGISTRY COPYRIGHT 2003 ACS on STN
RN 221679-24-9 REGISTRY
CN Glycine, (.beta.R)-N-ethyl-.beta.,3-dihydroxy-N-methyl-L-tyrosyl-L-valyl-3-
hydroxy-L-isoleucyl-, ethyl ester, cyclic (13.fwdarw.3)-ether (9CI) (CA
INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
MF C27 H42 N4 O8
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Russel 10_088078



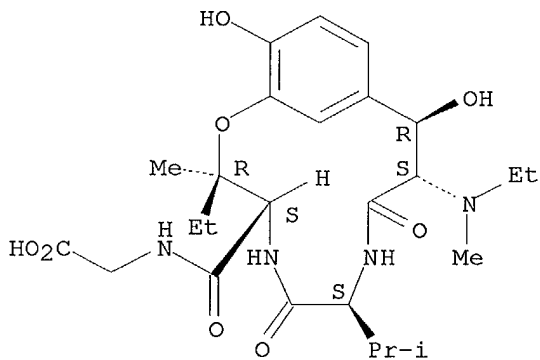
1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:252635

L3 ANSWER 4 OF 22 REGISTRY COPYRIGHT 2003 ACS on STN
RN 221679-23-8 REGISTRY
CN Glycine, (.beta.R)-N-ethyl-.beta.,3-dihydroxy-N-methyl-L-tyrosyl-L-valyl-3-hydroxy-L-isoleucyl-, cyclic (13.fwdarw.3)-ether (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
MF C25 H38 N4 O8
SR CA
LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:252635

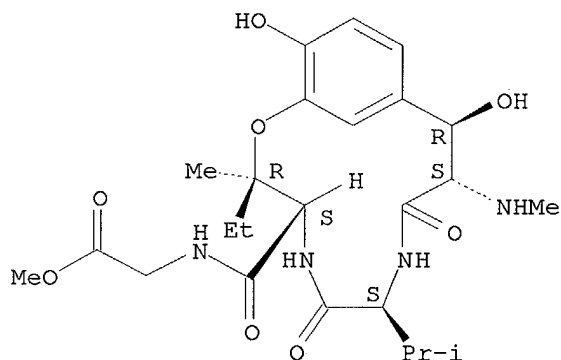
L3 ANSWER 5 OF 22 REGISTRY COPYRIGHT 2003 ACS on STN
RN 221679-22-7 REGISTRY
CN Glycine, (.beta.R)-.beta.,3-dihydroxy-N-methyl-L-tyrosyl-L-valyl-3-hydroxy-L-isoleucyl-, methyl ester, cyclic (13.fwdarw.3)-ether (9CI) (CA INDEX NAME)

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NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
MF C24 H36 N4 O8
SR CA
LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:252635

L3 ANSWER 6 OF 22 REGISTRY COPYRIGHT 2003 ACS on STN
RN 208392-87-4 REGISTRY
CN Glycine, (.beta.R)-.beta.,3-dihydroxy-N-methyl-L-tyrosyl-L-alanyl-3-hydroxy-L-isoleucyl-, cyclic (13.fwdarw.3)-ether (9CI) (CA INDEX NAME)

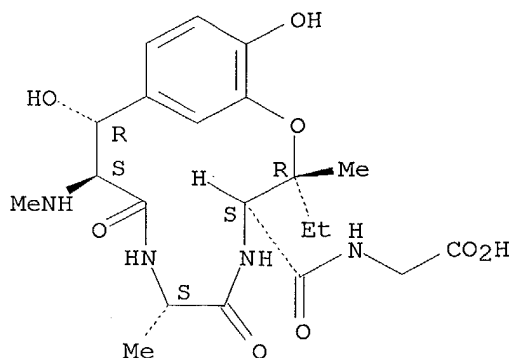
OTHER NAMES:

CN Ustiloxin F
FS PROTEIN SEQUENCE; STEREOSEARCH
MF C21 H30 N4 O8
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry. Rotation (-).

Russel 10_088078



3 REFERENCES IN FILE CA (1907 TO DATE)
3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:252635

REFERENCE 2: 129:41400

REFERENCE 3: 129:38537

L3 ANSWER 7 OF 22 REGISTRY COPYRIGHT 2003 ACS on STN

RN 207792-23-2 REGISTRY

CN 2-Oxa-5,8-diazabicyclo[10.3.1]hexadeca-1(16),12,14-triene-4-carboxamide,
3-ethyl-11,15-dihydroxy-N-(2-hydroxyethyl)-3-methyl-10-(methylethyl)-7-(1-
methylethyl)-6,9-dioxo-, (3R,4S,7S,10S,11R)- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

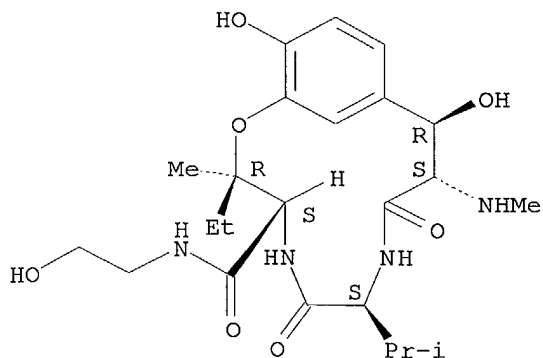
MF C23 H36 N4 O7

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

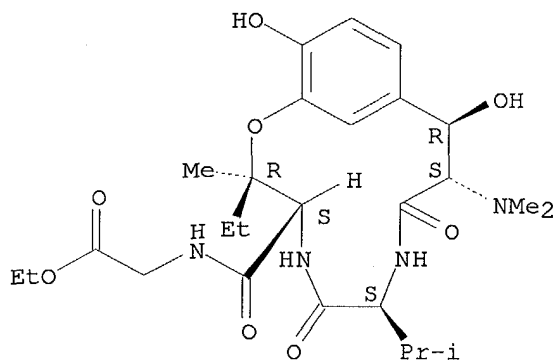
REFERENCE 1: 129:41400

Russel 10_088078

L3 ANSWER 8 OF 22 REGISTRY COPYRIGHT 2003 ACS on STN
RN 207792-21-0 REGISTRY
CN Glycine, (.beta.R)-.beta.,3-dihydroxy-N,N-dimethyl-L-tyrosyl-L-valyl-3-hydroxy-L-isoleucyl-, ethyl ester, cyclic (13.fwdarw.3)-ether (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
MF C26 H40 N4 O8
SR CA
LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:252635

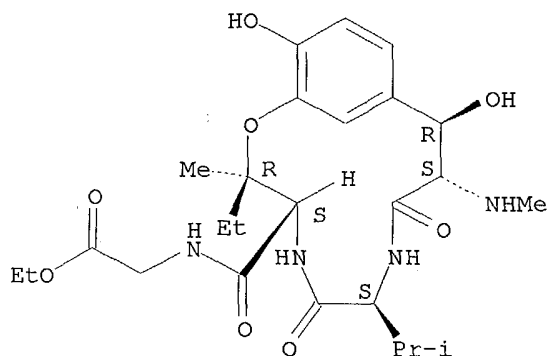
REFERENCE 2: 129:41400

L3 ANSWER 9 OF 22 REGISTRY COPYRIGHT 2003 ACS on STN
RN 207792-20-9 REGISTRY
CN Glycine, (.beta.R)-.beta.,3-dihydroxy-N-methyl-L-tyrosyl-L-valyl-3-hydroxy-L-isoleucyl-, ethyl ester, cyclic (13.fwdarw.3)-ether (9CI) (CA INDEX NAME)
FS PROTEIN SEQUENCE; STEREOSEARCH
MF C25 H38 N4 O8
SR CA
LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

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2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:252635

REFERENCE 2: 129:41400

L3 ANSWER 10 OF 22 REGISTRY COPYRIGHT 2003 ACS on STN

RN 175617-09-1 REGISTRY

CN Phomopsin D (9CI) (CA INDEX NAME)

OTHER NAMES:

CN L-Aspartic acid, 3-chloro-erythro-.beta.,5-dihydroxy-N-methyl-L-tyrosyl-3,4-didehydro-L-valyl-3-hydroxy-L-isoleucyl-3,4-didehydro-L-prolyl-(E)-2,3-didehydroisoleucyl-, cyclic (15.fwdarw.3)-ether

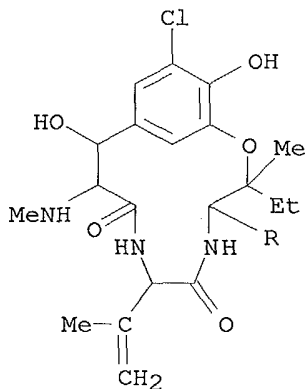
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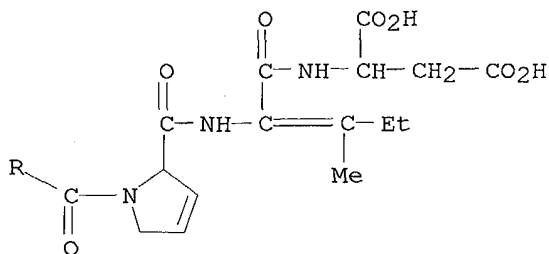
MF C36 H47 Cl N6 O12

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

PAGE 1-A





1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 124:315326

L3 ANSWER 11 OF 22 REGISTRY COPYRIGHT 2003 ACS on STN

RN 158274-98-7 REGISTRY

CN Glycine, (.beta.R)-.beta.,5-dihydroxy-2-[(R)-(2-hydroxyethyl)sulfinyl]-N-methyl-L-tyrosyl-L-valyl-3-hydroxy-L-isoleucyl-, cyclic (15.fwdarw.3)-ether (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2-Oxa-5,8-diazabicyclo[10.3.1]hexadecane, cyclic peptide deriv.

CN Glycine, threo-.beta.,5-dihydroxy-2-[(2-hydroxyethyl)sulfinyl]-N-methyl-L-tyrosyl-L-valyl-3-hydroxy-L-isoleucyl-, cyclic (15.fwdarw.3)-ether, (R)-

OTHER NAMES:

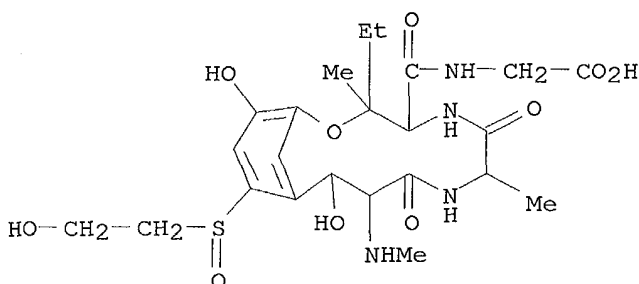
CN Ustiloxin C

FS PROTEIN SEQUENCE

MF C23 H34 N4 O10 S

SR CA

LC STN Files: CA, CANCERLIT, CAPLUS, MEDLINE, TOXCENTER



4 REFERENCES IN FILE CA (1907 TO DATE)
4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 129:41400

REFERENCE 2: 123:283737

REFERENCE 3: 123:25336

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REFERENCE 4: 121:225960

L3 ANSWER 12 OF 22 REGISTRY COPYRIGHT 2003 ACS on STN

RN 158243-18-6 REGISTRY

CN Glycine, (.beta.R)-.beta.,3-dihydroxy-N-methyl-L-tyrosyl-L-valyl-3-hydroxy-L-isoleucyl-, cyclic (13.fwdarw.3)-ether (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2-Oxa-5,8-diazabicyclo[10.3.1]hexadecane, cyclic peptide deriv.

CN Glycine, threo-.beta.,3-dihydroxy-N-methyl-L-tyrosyl-L-valyl-3-hydroxy-L-isoleucyl-, cyclic (13.fwdarw.3)-ether

OTHER NAMES:

CN Ustiloxin D

FS PROTEIN SEQUENCE; STEREOSEARCH

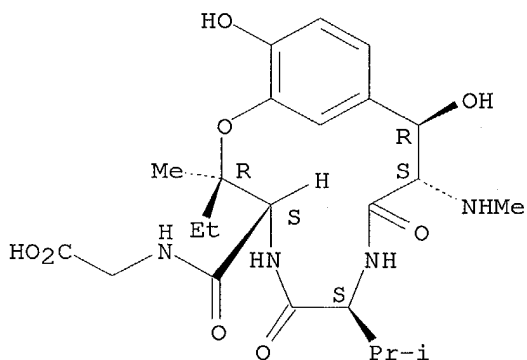
MF C23 H34 N4 O8

SR CA

LC STN Files: BIOBUSINESS, BIOSIS, CA, CANCERLIT, CAPLUS, CASREACT, MEDLINE, TOXCENTER

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

10 REFERENCES IN FILE CA (1907 TO DATE)

10 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 139:85641

REFERENCE 2: 136:200467

REFERENCE 3: 136:6316

REFERENCE 4: 134:17720

REFERENCE 5: 130:252635

REFERENCE 6: 129:41400

REFERENCE 7: 129:38537

REFERENCE 8: 123:283737

REFERENCE 9: 123:25336

REFERENCE 10: 121:225960

L3 ANSWER 13 OF 22 REGISTRY COPYRIGHT 2003 ACS on STN

RN 151841-41-7 REGISTRY

CN Glycine, (.beta.R)-2-[(R)-[(2S,4S)-4-amino-4-carboxy-2-hydroxybutyl]sulfinyl]-.beta.,5-dihydroxy-N-methyl-L-tyrosyl-L-alanyl-3-hydroxy-L-isoleucyl-, cyclic (15.fwdarw.3)-ether (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2-Oxa-5,8-diazabicyclo[10.3.1]hexadecane, cyclic peptide deriv.

CN Glycine, 2-[(4-amino-4-carboxy-2-hydroxybutyl)sulfinyl]-threo-.beta.,5-dihydroxy-N-methyl-L-tyrosyl-L-alanyl-3-hydroxy-L-isoleucyl-, cyclic (15.fwdarw.3)-ether, [2S-[1(S*),2R*,4R*]]-

OTHER NAMES:

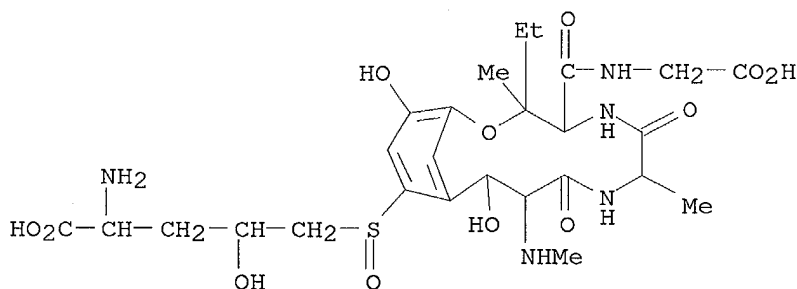
CN Ustiloxin B

FS PROTEIN SEQUENCE

MF C26 H39 N5 O12 S

SR CA

LC STN Files: BIOBUSINESS, BIOSIS, CA, CAPLUS, TOXCENTER



6 REFERENCES IN FILE CA (1907 TO DATE)

6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 129:41400

REFERENCE 2: 129:38537

REFERENCE 3: 126:264317

REFERENCE 4: 123:25336

REFERENCE 5: 121:225960

REFERENCE 6: 120:14886

L3 ANSWER 14 OF 22 REGISTRY COPYRIGHT 2003 ACS on STN

RN 151586-09-3 REGISTRY

CN Glycine, 2-[[4-(acetamino)-4-carboxy-2-hydroxybutyl]sulfinyl]-threo-.beta.,5-dihydroxy-N-methyl-L-tyrosyl-L-valyl-3-hydroxy-L-isoleucyl-, cyclic (15.fwdarw.3)-ether, disodium salt, [2S-[1(S*),2R*,4R*]]- (9CI)

Russel 10 088078

(CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2-Oxa-5,8-diazabicyclo[10.3.1]hexadecane, cyclic peptide deriv.

FS PROTEIN SEQUENCE

MF C30 H45 N5 O13 S . 2 Na

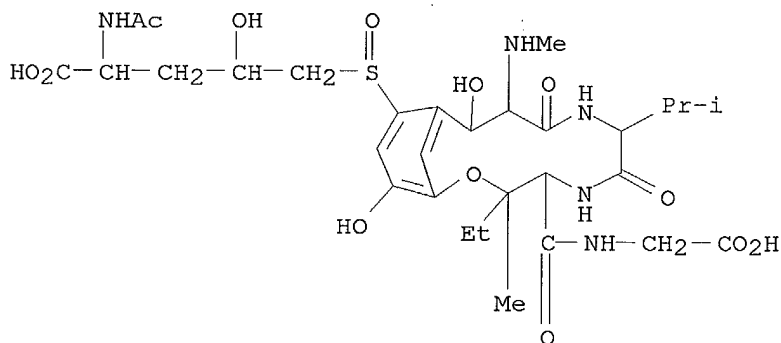
SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

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**RELATED SEQUENCES AVAILABLE WITH SEQLINK**

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●₂ Na

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 120:14886

L3 ANSWER 15 OF 22 REGISTRY COPYRIGHT 2003 ACS on STN

RN 151586-08-2 REGISTRY

CN Glycine, 2-[(4-amino-2-hydroxy-5-methoxy-5-oxopentyl)sulfinyl]-threo-
.beta.,5-dihydroxy-N-methyl-L-tyrosyl-L-valyl-3-hydroxy-L-isoleucyl-,
methyl ester, cyclic (15.fwdarw.3)-ether, dihydrochloride,
[2S-[1(S*),2R*,4R*]]- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2-Oxa-5,8-diazabicyclo[10.3.1]hexadecane, cyclic peptide deriv.

OTHER NAMES:

CN Ustiloxin A dimethyl ester dihydrochloride

FS PROTEIN SEQUENCE

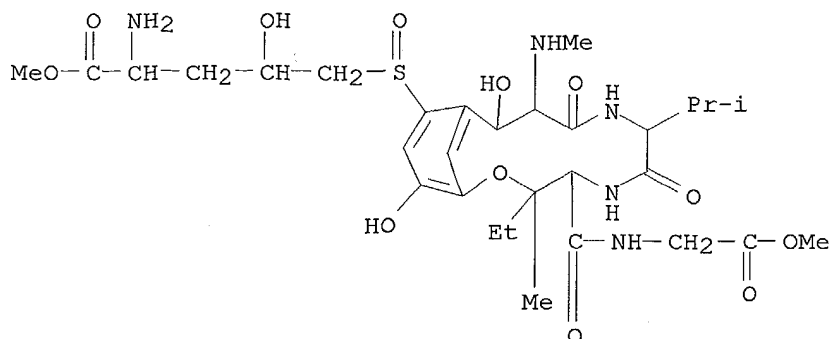
MF C30 H47 N5 O12 S . 2 Cl H

SR CA

LC STN Files: CA, CAPLUS, TOXCENTER

RELATED SEQUENCES AVAILABLE WITH SEOLINK

Russel 10_088078



● 2 HCl

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 120:14886

L3 ANSWER 16 OF 22 REGISTRY COPYRIGHT 2003 ACS on STN

RN 143557-93-1 REGISTRY

CN Glycine, (.beta.R)-2-[(R)-[(2S,4S)-4-amino-4-carboxy-2-hydroxybutyl]sulfinyl]-.beta.,5-dihydroxy-N-methyl-L-tyrosyl-L-valyl-3-hydroxy-L-isoleucyl-, cyclic (15.fwdarw.3)-ether (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2-Oxa-5,8-diazabicyclo[10.3.1]hexadecane, cyclic peptide deriv.

CN Glycine, 2-[(4-amino-4-carboxy-2-hydroxybutyl)sulfinyl]-threo-.beta.,5-dihydroxy-N-methyl-L-tyrosyl-L-valyl-3-hydroxy-L-isoleucyl-, cyclic (15.fwdarw.3)-ether, [2S-[1(S*),2R*,4R*]]-

OTHER NAMES:

CN Ustiloxin A

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C28 H43 N5 O12 S

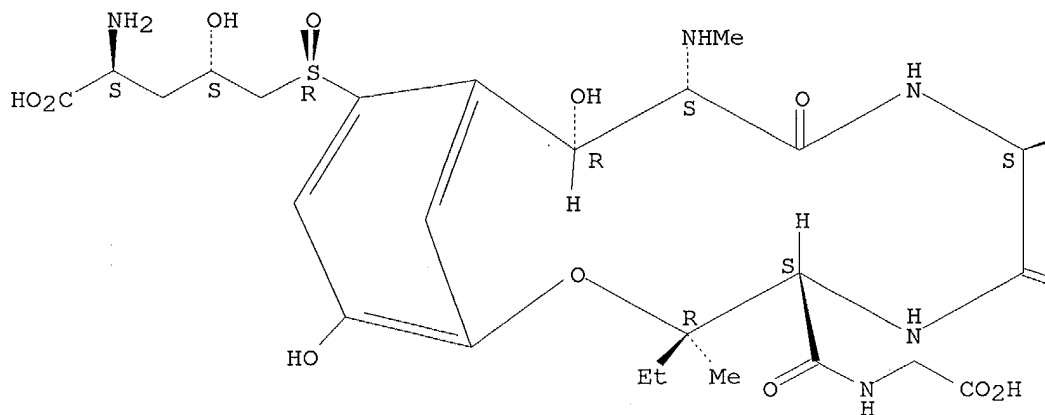
SR CA

LC STN Files: BEILSTEIN*, BIOSIS, CA, CANCERLIT, CAPLUS, MEDLINE, TOXCENTER
(*File contains numerically searchable property data)

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

Pr-i

= O

14 REFERENCES IN FILE CA (1907 TO DATE)
14 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE	1:	134:17720
REFERENCE	2:	129:41400
REFERENCE	3:	129:38537
REFERENCE	4:	126:264317
REFERENCE	5:	123:25336
REFERENCE	6:	121:225960
REFERENCE	7:	121:198163
REFERENCE	8:	121:73249
REFERENCE	9:	121:52013

REFERENCE 10: 121:256

L3 ANSWER 17 OF 22 REGISTRY COPYRIGHT 2003 ACS on STN
 RN 127102-34-5 REGISTRY
 CN Phomopsin A, dimer (9CI) (CA INDEX NAME)
 OTHER CA INDEX NAMES:
 CN 2-Oxa-5,8-diazabicyclo[10.3.1]hexadecane, cyclic peptide deriv.
 FS PROTEIN SEQUENCE; STEREOSEARCH
 MF (C36 H45 Cl N6 O12)2
 CI PMS, COM
 SR CA

RELATED SEQUENCES AVAILABLE WITH SEQLINK

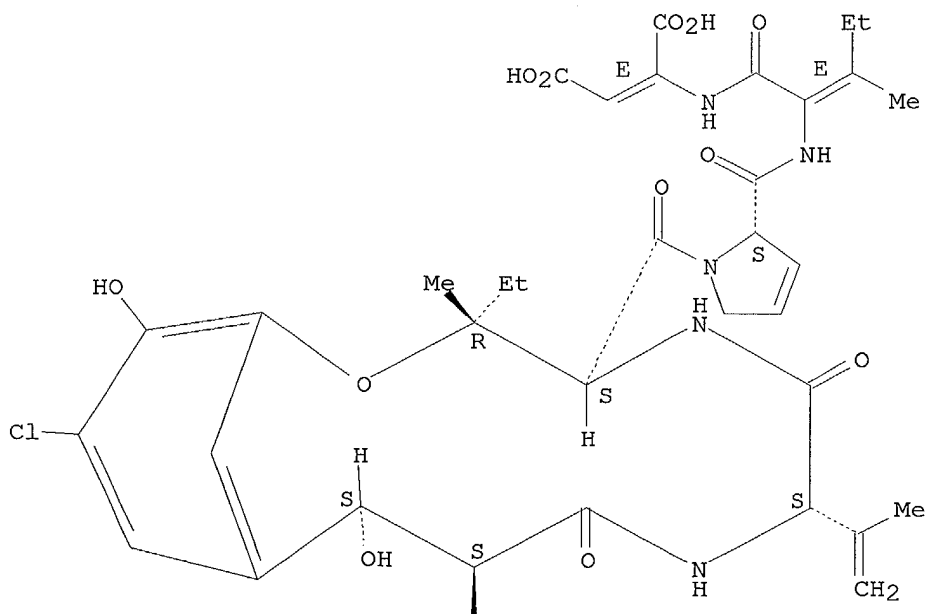
CM 1

CRN 64925-80-0
 CMF C36 H45 Cl N6 O12

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.
 Double bond geometry as shown.

PAGE 1-A



PAGE 2-A

NHMe

L3 ANSWER 18 OF 22 REGISTRY COPYRIGHT 2003 ACS on STN
RN 126061-17-4 REGISTRY
CN Phomopsin A, dimer, pentahydrate (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 2-Oxa-5,8-diazabicyclo[10.3.1]hexadecane, cyclic peptide deriv.
FS PROTEIN SEQUENCE; STEREOSEARCH
MF (C36 H45 Cl N6 O12)2 . 5 H2 O
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

RELATED SEQUENCES AVAILABLE WITH SEQLINK

CM 1

CRN 127102-34-5
CMF (C36 H45 Cl N6 O12)2
CCI PMS

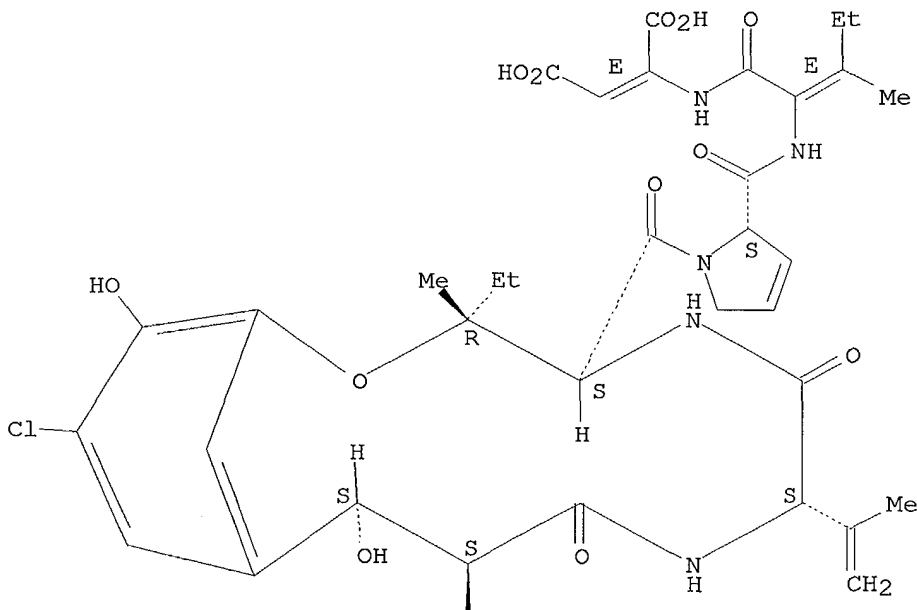
CM 2

CRN 64925-80-0
CMF C36 H45 Cl N6 O12

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.
Double bond geometry as shown.

PAGE 1-A





1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 112:158910

L3 ANSWER 19 OF 22 REGISTRY COPYRIGHT 2003 ACS on STN

RN 110580-02-4 REGISTRY

CN Aspartic acid, 1-[[(3R,4S,7S,10S,11R)-14-chloro-3-ethyl-11,15-dihydroxy-3-methyl-10-(methylamino)-7-(1-methylethyl)-6,9-dioxo-2-oxa-5,8-diazabicyclo[10.3.1]hexadeca-1(16),12,14-trien-4-yl]carbonyl]-L-prolylisoleucyl- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2-Oxa-5,8-diazabicyclo[10.3.1]hexadecane, DL-aspartic acid deriv.

CN DL-Aspartic acid, N-[N-[1-[[14-chloro-3-ethyl-11,15-dihydroxy-3-methyl-10-(methylamino)-7-(1-methylethyl)-6,9-dioxo-2-oxa-5,8-diazabicyclo[10.3.1]hexadeca-1(16),12,14-trien-4-yl]carbonyl]-L-prolyl]-DL-isoleucyl]-, [3R-(3R*,4S*,7S*,10S*,11R*)]-

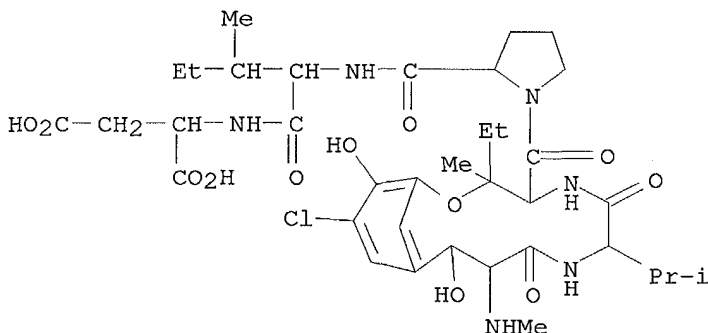
FS PROTEIN SEQUENCE

MF C36 H53 Cl N6 O12

SR CA

LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER
(*File contains numerically searchable property data)

RELATED SEQUENCES AVAILABLE WITH SEQLINK



2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 134:261242

REFERENCE 2: 107:168352

L3 ANSWER 20 OF 22 REGISTRY COPYRIGHT 2003 ACS on STN

RN 89085-54-1 REGISTRY

CN 1-5-Phomopsin A, 5-[(2E)-2,3-didehydroisoleucinamide]- (9CI) (CA INDEX

Russel 10_088078

NAME)

OTHER CA INDEX NAMES:

CN Phomopsin A, 5-[(E)-2,3-didehydroisoleucinamide]-6-de[(E)-2,3-didehydroaspartic acid]-

OTHER NAMES:

CN Isoleucinamide, 3-chloro-erythro-.beta.,5-dihydroxy-N-methyl-L-tyrosyl-3,4-didehydro-L-valyl-3-hydroxy-L-isoleucyl-3,4-didehydro-L-prolyl-2,3-didehydro-, cyclic (15.fwdarw.3)-ether, (E)-

CN Phomopsinamine A

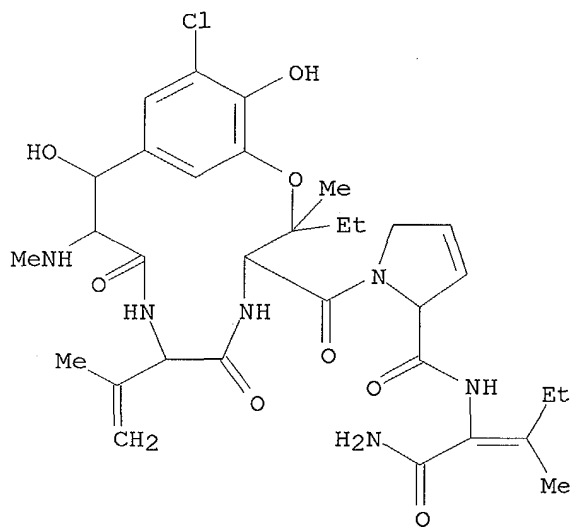
FS PROTEIN SEQUENCE

MF C32 H43 Cl N6 O8

LC STN Files: BEILSTEIN*, CA, CAPLUS, TOXCENTER

(*File contains numerically searchable property data)

Currently available stereo shown.



4 REFERENCES IN FILE CA (1907 TO DATE)

4 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 134:261242

REFERENCE 2: 107:168352

REFERENCE 3: 107:40303

REFERENCE 4: 100:103882

L3 ANSWER 21 OF 22 REGISTRY COPYRIGHT 2003 ACS on STN

RN 64925-81-1 REGISTRY

CN Phomopsin B (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2-Oxa-5,8-diazabicyclo[10.3.1]hexadecane, phomopsin A deriv.

CN Phomopsin A, 1-(erythro-.beta.,3-dihydroxy-N-methyl-L-tyrosine)-

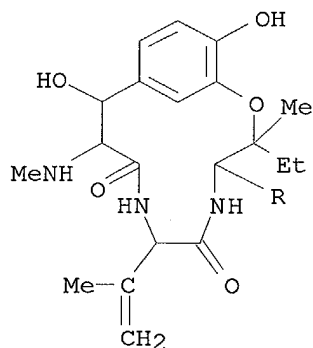
OTHER NAMES:

Russel 10_088078

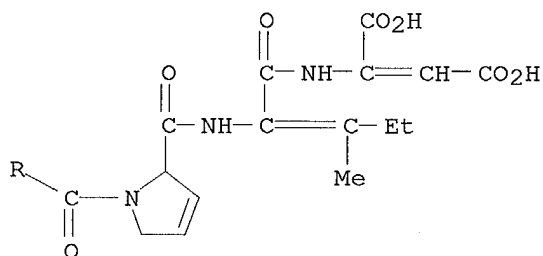
CN Aspartic acid, erythro-.beta.,3-dihydroxy-N-methyl-L-tyrosyl-3,4-didehydro-L-valyl-3-hydroxy-L-isoleucyl-3,4-didehydro-L-prolyl-(E)-2,3-didehydroisoleucyl-(E)-2,3-didehydro-, cyclic (13.fwdarw.3)-ether
FS PROTEIN SEQUENCE
MF C36 H46 N6 O12
LC STN Files: CA, CAPLUS, TOXCENTER

RELATED SEQUENCES AVAILABLE WITH SEQLINK

PAGE 1-A



PAGE 2-A



6 REFERENCES IN FILE CA (1907 TO DATE)
6 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 136:279676
REFERENCE 2: 130:252635
REFERENCE 3: 111:2426
REFERENCE 4: 107:168352
REFERENCE 5: 105:55741
REFERENCE 6: 88:16986

L3 ANSWER 22 OF 22 REGISTRY COPYRIGHT 2003 ACS on STN

RN 64925-80-0 REGISTRY

CN Phomopsin A (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

CN 2-Oxa-5,8-diazabicyclo[10.3.1]hexadecane, cyclic peptide deriv.

OTHER NAMES:

CN 3-Chloro-erythro-.beta.,5-dihydroxy-N-methyl-L-tyrosyl-3,4-didehydro-L-valyl-3-hydroxy-L-isoleucyl-3,4-didehydro-L-prolyl-(E)-2,3-didehydroisoleucyl-(E)-2,3-didehydroaspartic acid cyclic (15.fwdarw.3)-ether

CN Aspartic acid, 3-chloro-erythro-.beta.,5-dihydroxy-N-methyl-L-tyrosyl-3,4-didehydro-L-valyl-3-hydroxy-L-isoleucyl-3,4-didehydro-L-prolyl-(E)-2,3-didehydroisoleucyl-(E)-2,3-didehydro-, cyclic (15.fwdarw.3)-ether

CN NSC 381839

FS PROTEIN SEQUENCE; STEREOSEARCH

DR 126061-16-3

MF C36 H45 Cl N6 O12

CI COM

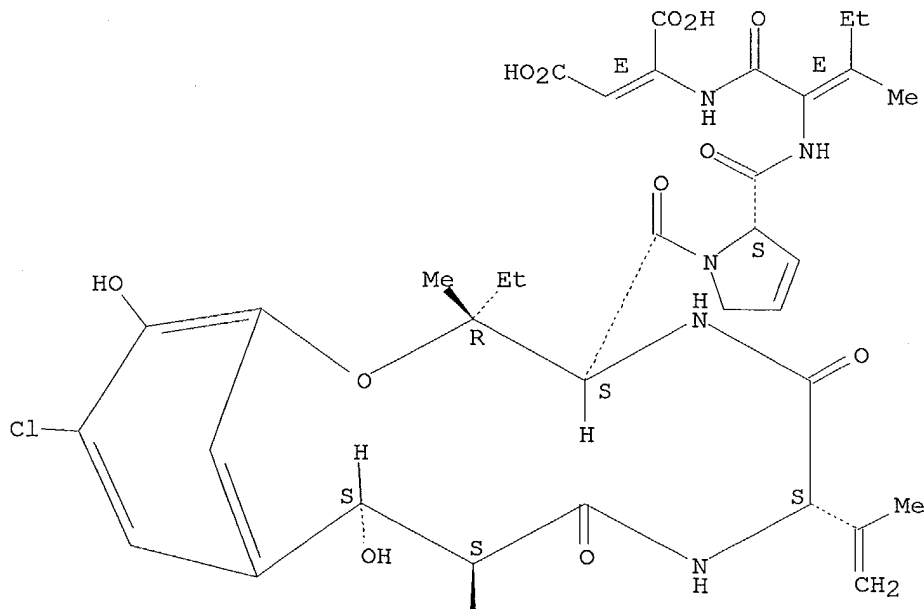
LC STN Files: AGRICOLA, ANABSTR, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAPLUS, CHEMCATS, CSCHEM, DDFU, DRUGU, EMBASE, MEDLINE, NAPRALERT, RTECS*, TOXCENTER, VETU
(*File contains numerically searchable property data)

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

Double bond geometry as shown.

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Russel 10_088078

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1
NHMe

49 REFERENCES IN FILE CA (1907 TO DATE)
49 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE	1:	136:279676
REFERENCE	2:	134:261242
REFERENCE	3:	134:17720
REFERENCE	4:	133:164285
REFERENCE	5:	131:337315
REFERENCE	6:	131:130273
REFERENCE	7:	130:252635
REFERENCE	8:	130:152150
REFERENCE	9:	126:327140
REFERENCE	10:	124:315326